Ab initio many-body calculations of the ^{4}He photo-absorption cross section

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Abstract

A major goal of nuclear theory is to make quantitative calculations of low-energy nuclear observables starting from microscopic internucleon forces. Computationally, this is complicated by the large model spaces needed to reach convergence in many-body approaches, such as the no-core shell model (NCSM). In recent years, the similarity renormalization group (SRG) has provided a powerful and versatile means to soften interactions for *ab initio* structure calculations, thus leading to convergence within smaller model spaces. Here we compute the ^{4}He total photo absorption cross section and study, for the first time, the consistency of the SRG approach in a continuum observable.

I. INTRODUCTION

The increased power of supercomputers has stimulated the development of new algorithms to solve the nuclear many-body problem. The *ab initio* no-core shell-model (NCSM) [1] is one such method in which all nucleons are taken to be active, a practice generally restricted to few-body systems because the number of many-nucleon states quickly becomes unmanageable. The intrinsic nonrelativistic Hamiltonian for a system of A protons and neutrons is [2]

$$\hat{\mathrm{H}} = \frac{1}{A}\sum_{i<j}\frac{(\vec{p}_i - \vec{p}_j)^2}{2M_N} + \sum_{i>j}^{A} V_{ij}^{NN} + \sum_{i>j>k}^{A} V_{ijk}^{NNN} + \ldots, \tag{1}$$

where V_{ij}^{NN} and V_{ijk}^{NNN} are the two- and three-nucleon interactions respectively, which can depend on the relative coordinates and momenta for nonlocal forces between particles, $\vec{p}_i$ is the momentum of particle i, and M_N is the nucleon mass. One then diagonalizes this Hamiltonian in a many-body basis. We use a translationally invariant harmonic oscillator (HO) basis [3], which depends only on Jacobi relative coordinates.This has the unique advantage to allow for easy separation of center of mass motion from the internal degrees of freedom [1]. The NCSM, in principle, provides the exact solution to the Hamiltonian in Eq. 1. In practice, we truncate the size of the HO basis at a finite value characterized by the parameter $N_{\max}$.

Initially, two-nucleon (NN) interactions built on phenomenological ground to fit the wealth of nucleon-nucleon experimental data were used for calculations and generally gave a good description for low-energy NN data. However, it quickly became apparent that the properties of heavier systems cannot be described without the inclusion of NNN, or higher, interactions, and constructing such higher-order forces in a consistent way is not feasible without a solid theoretical foundation. At the same time, a direct description of nuclear forces from the underlying theory of quantum chromodynamics (QCD) is not yet feasible due to the non-perturbative nature of this theory at the low energies relevant for nuclear physics. We use forces derived in the framework of chiral effective field theory (χEFT), an effective theory of QCD, which offers a systematic and model independent way to describe higher-order forces [4].

Numerically, convergence in the truncated model space is difficult to achieve because the bare nuclear interaction strongly couples high- and low-momentum components, which in

local interactions looks like a "hard core". The usual scheme to alleviate this problem is based on a unitary transformation of the Hamiltonian [5]. As a result of this process, the model space is decoupled from the excluded part of the Hamiltonian, essentially softening the hard core of the interaction. Such transformation have been used to great effect in a range of nuclear physics problems [1, 6–9]. In this work we use the similarity renormalization group (SRG) method to achieve a partial decoupling [10].

A drawback of effective interactions is that any transformation that softens the hard core will induce higher order interactions. The SRG method offers an approach that preserves the hierarchy observed in the initial χEFT forces (ie. NN>NNN> ...) that we use to describe the interaction between nucleons. Prior evidence suggests that SRG improves the convergence properties of the evolved many-body calculations of nuclear structure [6, 10]. However, a similar study is still missing for calculations of nuclear reactions, specifically the dipole response and sum rule.

Calculating reaction observables, such as a nuclear photo-absorption cross section, within an *ab initio* framework requires the evaluation of many-body scattering states, which cannot be described by expansions over square-integrable basis states such as those used in the NCSM. However, one can avoid this obstacle by using the Lorentz integral transform (LIT) approach to map the continuum problem into a bound state problem [11], which can be solved by means of typical bound state techniques.

The *ab initio* NCSM, along with the LIT method, have been successfully applied to the computation of electromagnetic response functions of the ^{4}He nucleus [12]. For the ^{4}He photo absorption cross section in particular, previous work [13] using effective interactions obtained with the Lee-Suzuki unitary transformation [14, 15] has proven successful in describing this reaction starting from χEFT NN+NNN interactions. Other bound state techniques have also been successfully combined with the LIT method to compute cross sections. The effective interaction hyperspherical harmonic (EIHH) [16, 17], an accurate bound state approach similar to the NCSM, has been useful when examining reactions involving six- [18, 19] and seven-body [20] nuclei with NN potentials. Our approach differs from the previous work in that we compute reaction observables using realistic NN+NNN interactions from χEFT in combination with the SRG method to renormalize the Hamiltonian of our system.

Section II provides background on the approach we use to compute the total photo-absorption cross section. In particular, we discuss how the SRG method modifies the Hamil-

tonian of our system and how the LIT can be used to compute the response induced by the an external perturbation, in our case, the dipole operator. In section III we describe our results in three parts: convergence of the observables we compute with respect to the size of the NCSM model space adopted, a discussion on the unitarity of the SRG transformation in our context and a comparison to experimental cross section data. Lastly, section IV gives a brief summary of our results and describes the next steps in this research.

II. APPROACH

The aim of the present work is to examine the performance and consistency of the SRG method when applied to a continuum observable, in particular, the total photo-absorption cross section. At low excitation energies the nuclear photo-absorption process can be described by the cross section [21]

$$\sigma_\gamma(\omega) = 4\pi^2 \frac{e^2}{\hbar c} \omega R(\omega), \tag{2}$$

where ω is the perturbing photon energy. Here, $R(\omega)$ is the inclusive response function

$$R(\omega) = \int d\Psi_f \left| \langle \Psi_f | \hat{D} | \Psi_0 \rangle \right|^2 \delta(E_f - E_0 - \omega), \tag{3}$$

where E_f and E_0 represent the final and initial state energies along with their associated wavefunctions, $|\Psi_f\rangle$ and $|\Psi_0\rangle$, respectively and $\hat{D}$ is the dipole operator given by

$$\hat{D} = \sqrt{\frac{4\pi}{3}} \sum_{i=1}^{A} \frac{\tau_i^z}{2} r_i Y_{10}(\vec{r}_i). \tag{4}$$

To obtain the total cross section we: (i) solve the many-body Schrödinger equation for the ground state, $|\Psi_0\rangle$, of ^{4}He, and obtain the inclusive response, Eq. (3) by (ii) evaluation [22] and (iii) inversion [23] of its integral transform with a Lorentzian kernel, described in more detail below, and (iv) calculate the photo-absorption cross section using Eq. (2). We perform the first two steps in the framework of the *ab initio* NCSM [1]. In this method the eigenstates and the eigenvalues of the Hamiltonian are obtained by diagonalization in Hilbert space spanned by a complete set of harmonic oscillator (HO) basis states. These states are truncated at a maximum excitation of $N_{max}\hbar\Omega$ above the minimum energy configuration, where Ω is the HO frequency. The description of the two- and three-nucleon interactions are based on χEFT [24, 25].

Before we compute the ground state of ^{4}He we renormalize the Hamiltonian via the SRG method. As implemented for nuclear physics [10], this is a series of unitary transformations in momentum space, U_s, on the Hamiltonian of the system,

$$\hat{H}_s = \hat{U}_s \hat{H}_{s=0} \hat{U}_s^\dagger, \tag{5}$$

where s, running from zero to infinity, is a parameter which labels the sequence of Hamiltonians

Denoting T as the kinetic energy operator, these transformations can be implemented as a flow equation [26] in s,

$$\frac{dH_s}{ds} = \left[\left[T, H_s\right], H_s\right], \tag{6}$$

or, more commonly, in the momentum parameter, $\lambda = s^{-1/4}$, which starts at infinity and approaches zero as the flow equation is evaluated. As the transformation is performed, λ proceeds to zero (or s increases), the momentum space Hamiltonian is driven to a band diagonal form [27] and its high- and low-momentum sectors decouple. The parameter λ is convenient because it represents the momentum scale at which the decoupling occurs. As a result, SRG-evolved Hamiltonians lead to faster convergence for many-body calculations of nuclear observables.

Transforming the Hamiltonian induces the appearance of higher order many-body forces. However, as a result of renormalization, as long as the initial forces used to construct the Hamiltonian follow a hierarchy of deceasing strength (NN>NNN> ...), so will the terms induced by the SRG method [6]. As we will show in section IV, including the higher order induced terms is important to preserve the unitary nature of the transformation without which results become dependent on the SRG flow parameter. Previous calculations suggest that evolving to $\lambda = 2.0$ fm^{-1} provides a good balance between improved convergence, from the decoupling of high- and low-momentum components, and growth of the induced many-body terms

To compute the inclusive cross section we need the inclusive response function given in Eq. 3. The LIT [22] obtains the response function, $R(\omega)$, after the evaluation and subsequent inversion [23] of its integral transform with a Lorentzian kernel of finite width,

$$L(\sigma_R, \sigma_I) = \int d\omega \frac{R(\omega)}{(\omega - \sigma_R)^2 + \sigma_I^2}. \tag{7}$$

Alternatively, the Lanczos algorithm [22] allows the LIT to be written as a continued fraction,

$$L(\sigma_R, \sigma_I) = \frac{\langle \Psi_0 | \hat{D}^\dagger \hat{D} | \Psi_0 \rangle}{\sigma_I} \mathrm{Im} \left(\frac{1}{z - a_0 - \dfrac{b_1^2}{z - a_1 - \ldots}} \right), \tag{8}$$

where the a_n and b_n are the Lanczos coefficients and $z = E_0 + \sigma_R + \sigma_I$. The quantity $\langle \Psi_0 | \hat{D}^\dagger \hat{D} | \Psi_0 \rangle$ is the total strength of the transition induced by the dipole operator. The response function, $R(\omega)$, can then be obtained by the inversion of the integral transform of Eq. 7.

III. RESULTS

We are interested in the convergence of three observables: the ground state energy, the root mean square (RMS) radius and the total dipole strength of ^{4}He. For our calculations we use the same SRG evolution scheme as Ref. [6], summarized in Table I. In this scheme we obtain separate NN and NNN parts of the nuclear interaction. This allows us to examine the effects on the nuclear observables when using a combination of initial or SRG-evolved NN and NNN interactions. To achieve this, the A = 2 subsystem is evolved first, giving us the NN part of the SRG-evolved interaction. Then the A = 3 subsystem is evolved to determine the combined NN+NNN interaction. One can then isolate the NNN part by subtracting the previously computed NN part. Having obtained the separate two- and three-body parts, one can apply them in various combinations.

TABLE I: Definitions of the various calculations

NN-only:	No initial NNN interaction
	and do not keep NNN-induced interaction
NN+NNN-induced:	No initial NNN interaction
	and keep NNN-induced interaction
NN+NNN:	Include an initial NNN interaction
	and keep NNN-induced interaction

Fig. 1 shows, for $\hbar\Omega = 28$ MeV and $\lambda = 2.0$ fm^{-1}, the ground state energy starts to

converge around $N_{\max} = 10$. The inclusion of the initial NNN interaction increases the binding energy of the system. Accidentally, the NN-only converged energy is nearly the same value as the full NN+NNN calculation. This behaviour has been seen in previous work, and we will discuss this further when considering a range of λ values.

We observe a similar behaviour for the RMS radius and total dipole strength. Convergence occurs later than the ground state energy, around $N_{\max} = 14$ for the RMS radius and $N_{\max} = 18$ for the total dipole strength, but still within the size of our maximum model space. Both observables also follow a similar pattern to convergence. This should not be surprising considering the approximate relation between them [28]:

$$\langle \Psi_0 | \hat{D}^\dagger \hat{D} | \Psi_0 \rangle \approx \frac{\mathrm{ZN}}{3(\mathrm{A}-1)} \langle r^2 \rangle. \tag{9}$$

Based on these results, the principle benefit of using an SRG-evolved interaction is apparent: fast convergence for all of our observables can be achieved within our large, but still finite, model space.

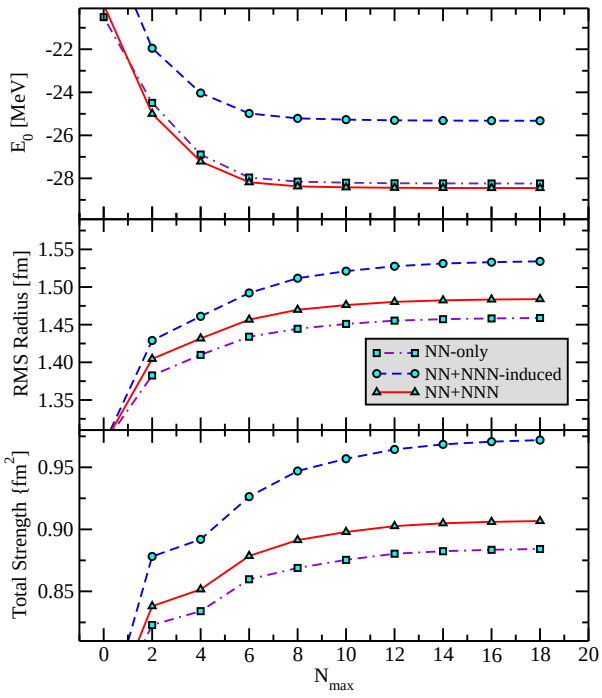

FIG. 1: Convergence of the ground state energy, E_0 (top panel), RMS radius, $\langle r^2 \rangle^{1/2}$ (middle panel) and total dipole strength, $\langle \Psi_0 | \hat{D}^\dagger \hat{D} | \Psi_0 \rangle$ (bottom panel) for NN-only, NN+NNN-induced and NN+NNN interactions. The calculations are performed in the model-space truncation $N_{\max}$ for $\hbar\Omega = 28$ MeV and SRG flow parameter $\lambda = 2.0$ fm^{-1}.

In Fig. 2, we study the dependence on the SRG evolution parameter on our three observables. The ground state energy, RMS radius and total dipole strength are plotted as a function of the SRG flow parameter, λ. The flow parameter starts at ∞ for the initial (or bare) interaction and is evolved toward $\lambda = 0$ fm^{-1}. The results in Fig. 2 where obtained with $\hbar\Omega = 28$ MeV and $N_{\max} = 18$ converged calculations. The ground state energy exhibits behaviour seen in previous work for the range of λ that we study. When we include the SRG induced three-body terms there is no dependence on λ between 1.8 fm^{-1} and 3.0 fm^{-1}. This behaviour is not influenced by the inclusion of an initial NNN interaction. As λ decreases below 1.8 fm^{-1} there is a slight drop in binding energy. This residual dependence on λ is due to missing four-body induced forces. Indeed, the importance of higher-order induced forces increases with decreasing values of λ. The shape of the NN-only curve, as described in Ref. [6], is caused by the way the SRG method affects the matrix elements of the Hamiltonian. Early in the evolution, the high-momentum matrix elements, the most repulsive, are most affected by the evolution. These matrix elements are rearranged into the induced NNN matrix elements, causing the binding energy to drop. As the evolution continues, lower momentum matrix elements, more attractive parts of the potential, are more affected, which causes the binding energy go back up. As a result, around $\lambda = 2$ fm^{-1}, NN-only and NN+NNN energies are, accidentally, close.

The other two observables clearly exhibit a dependence on λ. The NN+NNN-induced and NN+NNN curves follow the same pattern and the inclusion of an initial three-body force has no influence on the curve other than the shift to a lower value. The NN-only curve has a different shape form the others, but has the same general shape for both the RMS radius and total dipole strength.

Ideally, for a unitary transformation, one would expect no λ dependence, similar to what we see for the ground state energy. However, the transformation from initial Hamiltonian to effective Hamiltonian is equivalent to renormalizing the wavefunction in the Schrödinger equation,As a result, any operators we wish to study must either use the renormalized wavefunction or be transformed using the same unitary transformation as the Hamiltonian. For these calculations we use the bare r^2 and dipole operators, rather than their SRG-evolved counterparts. Also, similar to SRG-evolving the Hamiltonian, the evolution of the transition operators is further complicated by the fact that we must keep the higher order terms induced by the SRG method. We save this for future work with the hope that the λ

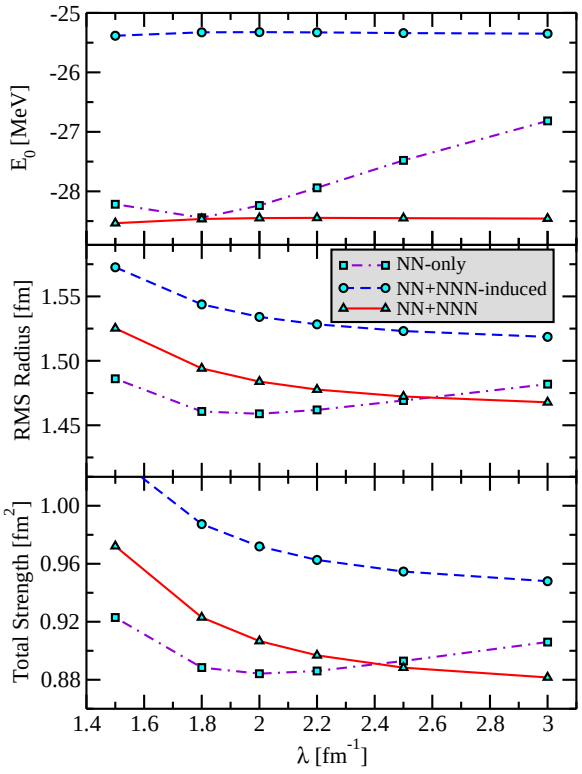

FIG. 2: Ground state energy, E_0 (top panel), RMS radius, $\langle r^2 \rangle^{1/2}$ (middle panel) and total dipole strength, $\langle \Psi_0 | \hat{D}^\dagger \hat{D} | \Psi_0 \rangle$ (bottom panel) as a function of SRG flow parameter, λ, for model-space truncation $N_{\max} = 18$ for $\hbar\Omega = 28$ MeV.

dependence will be mitigated for the RMS radius and total dipole strength.

Fig. 3 shows the photo-absorption cross section as a function of the photon energy, ω. The upper panel shows a range of λ values for NN+NNN-induced and the lower panel shows a comparison between NN+NNN-induced and NN+NNN. It is not surprising that we see a λ dependence in the cross section since we use the total dipole strength in its computation. For the higher values of λ, 2.5 fm^{-1} and 3.0 fm^{-1}, the dependence is somewhat mitigated, which is shown more clearly in the bottom panel for both NN+NNN-induced and NN+NNN. When compared to experimental data, shown in Fig. 4, we see that the total cross section is higher than most of the experimental results, NN+NNN-induced more so than NN+NNN. Generally, our best results are within the error bars of the recent Nakayama [29] results. However, only after SRG-evolving the dipole operator will we be able to draw a definitive conclusion.

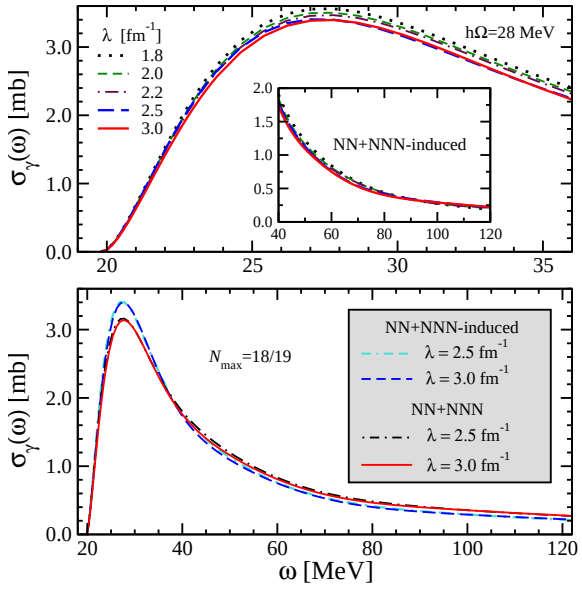

FIG. 3: The ^{4}He photo-absorption cross section, $\sigma_\gamma(\omega)$, as a function of energy, ω, for a range of λ values with the NN+NNN-induced interaction (top panel) and a comparison between NN+NNN-induced and NN+NNN (bottom panel). Both calculations use the model-space truncation $N_{\max} = 18$ for $\hbar\Omega = 28$ MeV.

IV. CONCLUSION

We have presented *ab initio* NCSM calculations using SRG-evolved two- and three-body forces from chiral effective field theory. Our primary goal was to examine the performance and consistency of the SRG method on the total dipole strength and the inclusive cross section of ^{4}He. We considered three important aspects in our calculations: convergence of the examined observables as size of the model space was increased, dependence of the observables on the SRG flow parameter, λ, and the effect of SRG evolution on the inclusive cross section.

Convergence of the ground state energy is achieved quickly, around $N_{max} = 10$, and is consistent with previous work. The RMS radius converges later than the ground state energy, but still before the largest model space we considered. The total dipole strength had the slowest convergence rate among the observables that we examined.

Ideally, changing the SRG flow parameter, λ, and thus, the amount of evolution the Hamiltonian receives, should not change the converged value of any observable. Previous

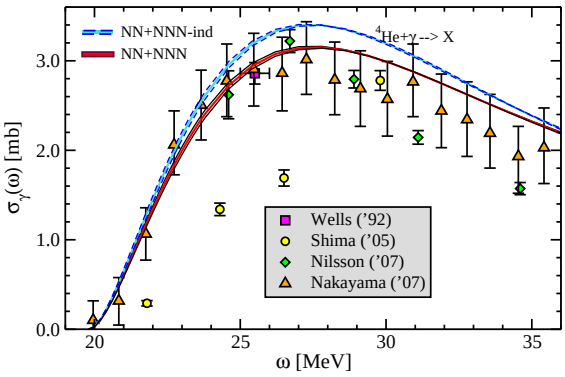

FIG. 4: The ^{4}He photo-absorption cross section as a function of excitation energy, ω, for NN+NNN-induced and NN+NNN interactions with a model-space truncation $N_{\max} = 18$ for $\hbar\Omega = 28$ MeV. Total cross section is compared to: Wells [30], Shima [31], Nilsson [32] and Nakayama [29].

work indicates that the higher-order many-body terms induced by SRG evolution become more important when increasing λ. We see this for the ground state energy when one includes the higher-body induced terms. However, for the other observables we see a clear dependence on λ even when we include the terms induced by evolving the Hamiltonian. This dependence comes from not evolving, and subsequently including the induced terms, the operators necessary for computing the observables, in particular, r^2 and the dipole operator, $\hat{D}$, given by Eq. 4.

For the total cross section it is not surprising that we see a clear dependence on λ based on the results for the total dipole strength. When compared to experimental data, our results tend to show larger values for the cross section. However, when including full NN+NNN interactions along with the three-body induced terms from the SRG evolution, our results are generally within the error bars of recent data by Nakayama [29]. we expect to see improvement in our inclusive cross section results by SRG evolving the dipole operator.

The next step for this work is fairly obvious. We must consistently evolve the operators responsible for the observables we wish to compute. However, evolution is not enough, we must also include the higher order induced terms in our calculations. Our next step is to see how the λ dependence is mitigated when computing the RMS radius. We will do this by SRG evolving the r^2 operator. If we see a mitigation in the dependence, similar to that of our ground state energy results, we will apply the same approach to the dipole operator to determine the effect on the total dipole strength and inclusive cross section.

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